

Supporting Information

A DFT-D study on the interaction between lactic acid and single-wall carbon nanotubes

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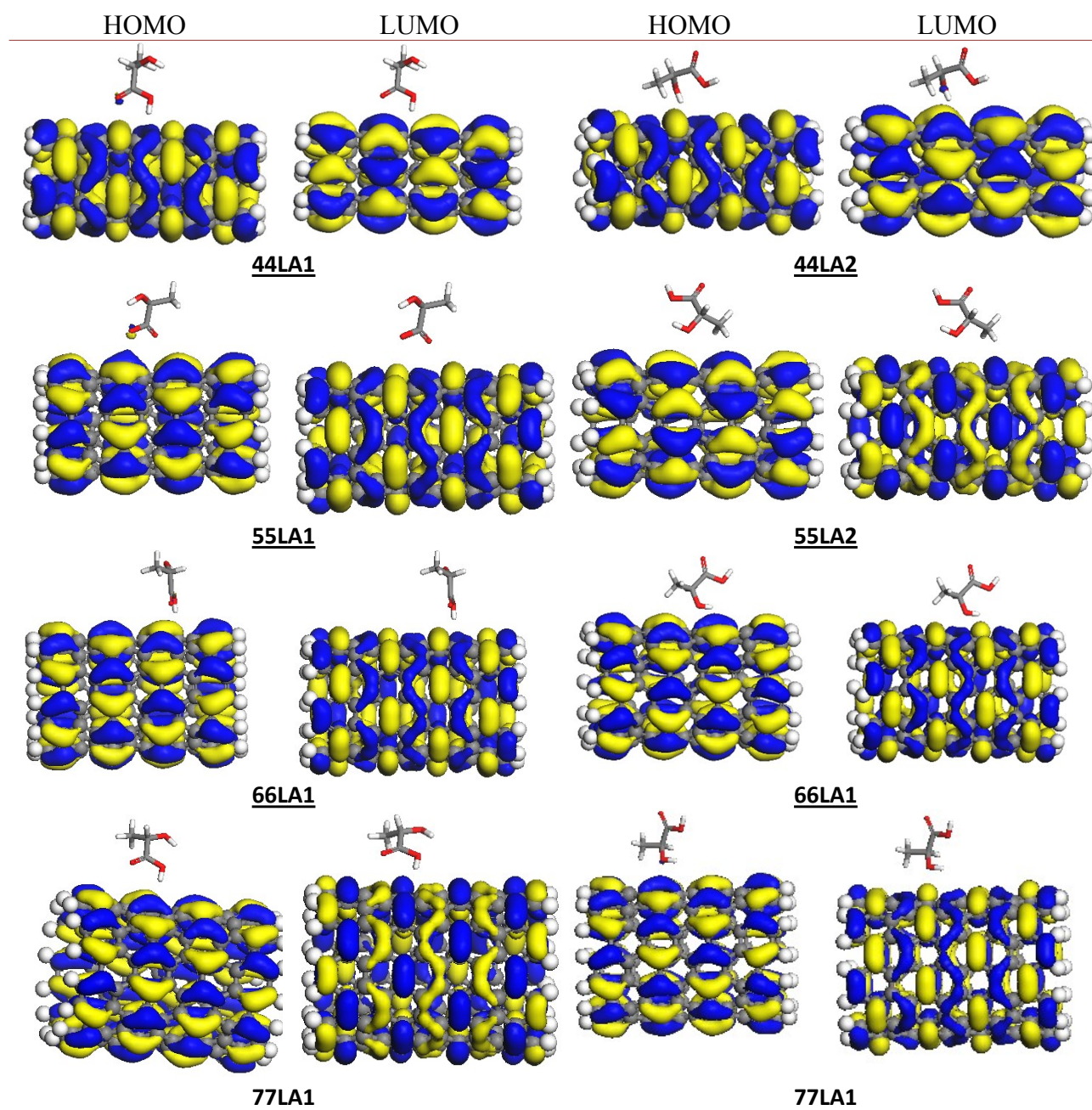


Fig. S1 Profiles of the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) for SWCNTs modified with lactic acid at DFT-D level of theory. The isovalue is taken as 0.03 au.

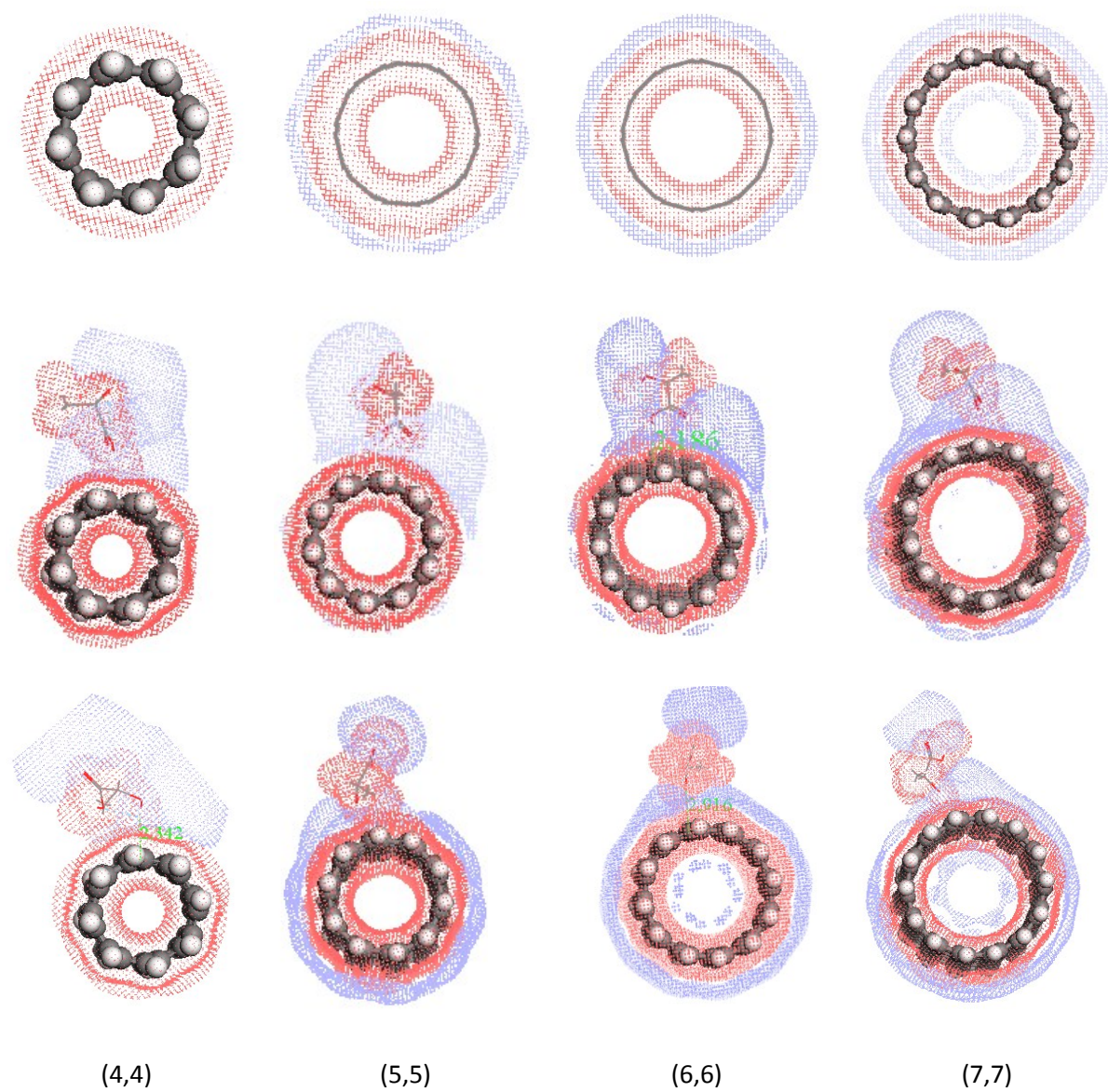


Fig. S2 MEP surfaces for the systems first row include SWCNTs, middle row show CNT complexes with LA in mode 1 and bottom row show CNT complexes with LA in mode 2. In the figure the blue color indicates the negative charge zone and the red color the positive charge zone, (red color with an isovalue = 0.04 au) and higher negative charge, (blue color with an isovalue = -0.03 au)